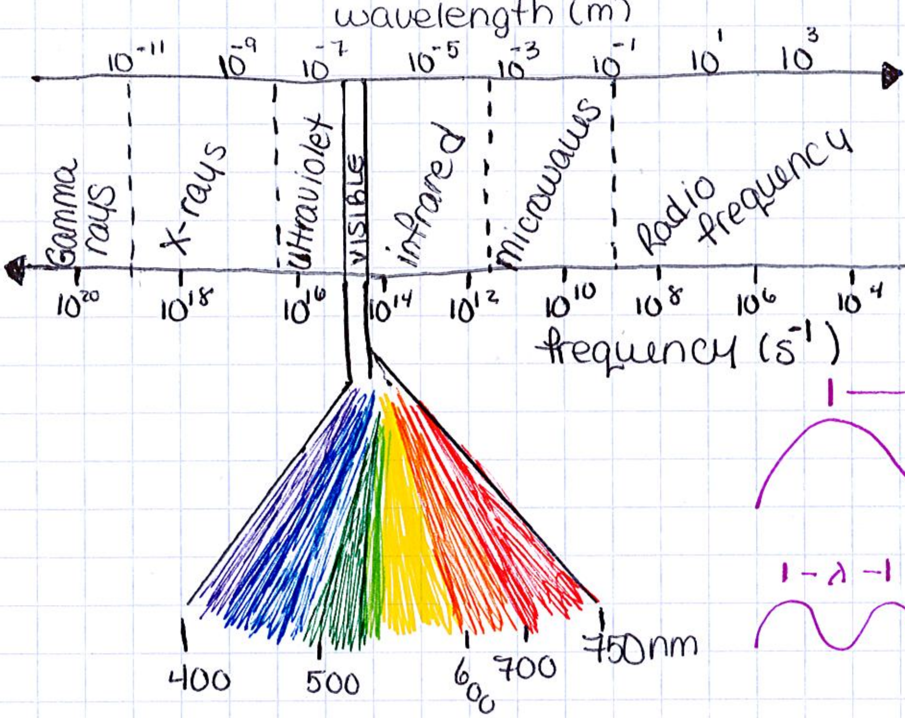
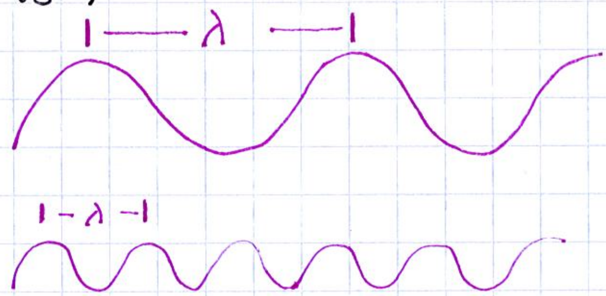
Ch 6: Electronic Structure of the Atom

1. The Wave Nature of Light - a lot of our understanding of the electronic structure of atoms comes from analyzing the light either emitted or absorbed by substances

A) electromagnetic radiation - (including visible light)





- has wave characteristics and propagates (moves) through a vacuum at the speed of light ($c = 3.00 \times 10^8$ m/s)

λ wavelength - distance between 2 peaks on a wave (m or nm or Å (angstrom) (10^{-10} m))

ν frequency - # cycles (waves) that pass a point per second ($^1/_s$, s^{-1}, or Hz)

λ and ν are inversely proportional as seen in the equation

$$c = \lambda \cdot \nu$$

$c = 3.00 \times 10^8$ m/s

Examples Conversions p14 $1 nm = 1 \times 10^{-9} m$

1) A laser used in eye surgery to fuse detached retinas produces radiation with a wavelength of 640.0nm. Calculate the frequency.

$c = \lambda \cdot \nu$

$c = 3.00 \times 10^{8} m/s$

$\lambda = 640.0 nm \left(\frac{1 m}{1 \times 10^{+9} nm}\right) = 6.400 \times 10^{-7} m$

$\nu = \frac{c}{\lambda} = \frac{3.00 \times 10^{8} m/s}{6.400 \times 10^{-7} m} = 4.69 \times 10^{14} Hz$

2) An FM radio station broadcasts EM radiation at a frequency of 103.4 MHz. Calculate the wavelength.

$103.4 MHz \left(\frac{1 \times 10^{6} Hz}{1 MHz}\right) = 1.034 \times 10^{8} Hz$

103,400,000

$\lambda = \frac{c}{\nu} = \frac{3.00 \times 10^{8} m/s}{1.034 \times 10^{8} 1/s} = 2.90 m$

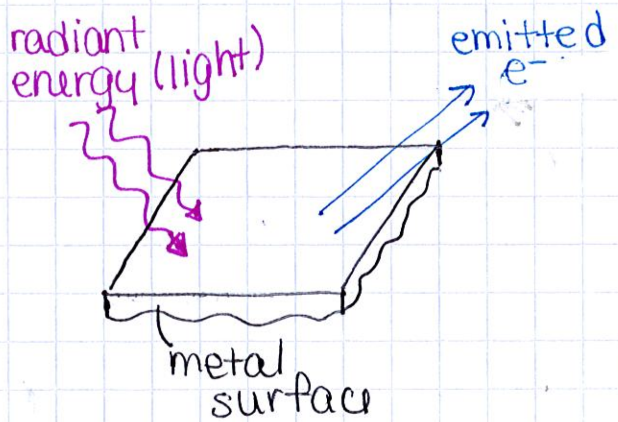
2. Quantized Energy & Photons

A) Heated objects give off radiation (red glow from a toaster or white light from an incandescent light bulb)

B) Energy can only be absorbed/emitted in discrete "chunks" called quantum

$E = h \cdot \nu$ $h = 6.626 \times 10^{-34} J \cdot s$ Planck's constant

C) The Photoelectric Effect & Photons



- Light shining on a clean metal surface causes the surface to emit e^-.
  - each metal does this at its own minimum frequency)
- Light hitting the surface is NOT acting like a wave, it acts like a stream of tiny energy packets (PHOTONS).

examples $E = h\nu$

3) A laser emits light with a frequency of 4.69×10^{14} Hz. What is the energy of one photon of radiation from this laser?

$$E = (6.626 \times 10^{-34}\ J \cdot s)(4.69 \times 10^{14}\ \tfrac{1}{s}) = 3.11 \times 10^{-19}\ J/photon$$

4) If the laser in #3 emits a pulse of energy containing 5.0×10^{17} photons, what is the total energy of the pulse?

$$5.0 \times 10^{17}\ photons\ (3.11 \times 10^{-19}\ J/photon) = .16\ J$$

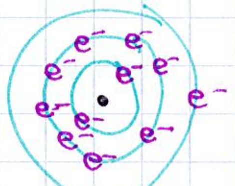
5) If the laser emits 1.3×10^{-2} J of energy, how many photons are released?

$$\frac{1.3 \times 10^{-2}\ J}{3.11 \times 10^{-19}\ J/photon} = 4.2 \times 10^{16}\ photons$$

3. What does all this mean for atoms? Line spectra & the Bohr model

- Elements under high voltage (like neon lights) emit colors of light w/specific wavelengths, called line spectrum.
  Figure 6.13 p219

- Bohr model of the atom - e^- move in circular orbits around the nucleus



Classical physics says that's impossible b/c electrically charged particles moving in circular paths continuously lose energy & spiral into the nucleus.
This does NOT happen!

- Only orbits of certain radii (w/specific energies) are permitted for an e^-.
- An e^- in an allowed orbit has a specific energy, it does not radiate or lose energy
- Energy can only be emitted/absorbed by the e^- as the e^- moves from one orbit (energy state) to another.

× Energy corresponding to each orbit:

$$E = (-hcR_H)\left(\frac{1}{n^2}\right) = -2.18\times10^{-18}\,J\left(\frac{1}{n^2}\right)$$

h = Planck's constant
c = speed of light
R_H = Rydberg constant = 1.096776×10^{7} 1/m)
n = energy level (orbit)

× Change in energy when an e^- moves between orbits:

$$\Delta E = E_f - E_i = E_{photon} = h\nu$$

$$\Delta E = h\nu = \frac{hc}{\lambda} = (-2.18\times10^{-18}\,J)\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

really only works for the e⁻ in a hydrogen atom

$-\Delta E$ = energy is emitted $+\Delta E$ = energy is absorbed

Examples

6) Calculate the energy of an electron in the hydrogen atom when n = 2.

$$E = -2.18\times10^{-18}\,J\left(\frac{1}{n^2}\right) = -2.18\times10^{-18}\,J\left(\frac{1}{2^2}\right)$$

$$= -5.45\times10^{-19}\,J$$

7) Calculate the change in energy when an electron moves from n = 4 to n = 1.

$$\Delta E = -2.18\times10^{-18}\,J\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$$= -2.18\times10^{-18}\,J\left(\frac{1}{1^2} - \frac{1}{4^2}\right) = -2.04\times10^{-18}\,J$$

8) Calculate the wavelength of radiation released when an electron moves from $n=6$ to $n=2$.

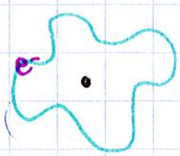
$$\Delta E = -2.18 \times 10^{-18} J \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = -2.18 \times 10^{-18} J \left(\frac{1}{2^2} - \frac{1}{6^2}\right) = -4.84 \times 10^{-19} J$$

$$\Delta E = \frac{hc}{\lambda} \qquad \lambda = \frac{hc}{\Delta E} = -4.11 \times 10^{-7}\ m$$

4. Matter Acting as a wave!

Suppose that the e^- orbiting the nucleus of a hydrogen atom could be a wave.

That wave would have a wavelength, which is dependent on the e^-'s mass



$$\lambda = \frac{h}{mv}$$

h = Planck's constant
mv = momentum (mass × velocity)

Example

9) Calculate the wavelength of an e^- moving with a speed of 5.97×10^6 m/s. The mass of an e^- is 9.11×10^{-31} kg. ($1 J = 1\ kg\,m^2/s^2$).

$$\lambda = \frac{6.626 \times 10^{-34} \frac{kg\,m^2}{s^2} \cdot s}{(9.11 \times 10^{-31}\ kg)(5.97 \times 10^6\ m/s)} = 1.22 \times 10^{-10}\ m$$

The dual nature of matter (wave-particle duality) limits how we can know both the exact location and momentum of of small objects like e⁻.

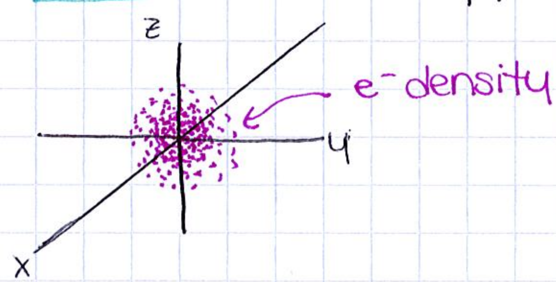
Heisenberg Uncertainty Principle see p. 224 for deeper explanation

It is inherently impossible to know both the exact location and momentum of an e⁻ in an atom simultaneously.

5. Quantum Mechanics & Orbitals

A) Erwin Schrödinger proposed an equation that takes into account both the wave-like and particle-like behavior of an electron. (New way of dealing w/ subatom particles called quantum mechanics)

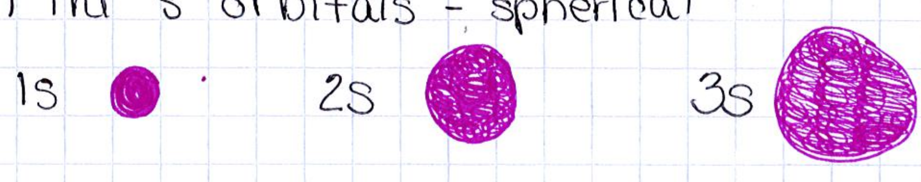
- treats an e⁻ like a standing circular wave around the nucleus (thru adv. calculus - functions called wave functions, Ψ)
- still uses Heisenberg's Uncertainty Principle, so scientists discuss the probability of finding an e⁻, or electron density, Ψ^2.



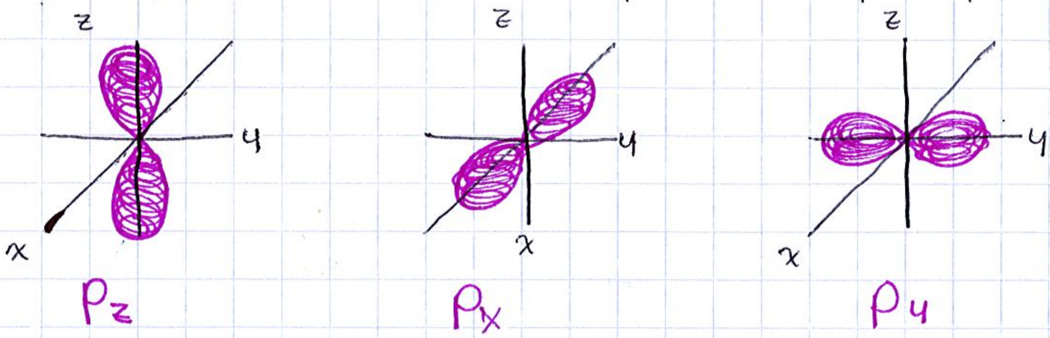
B) Orbitals - solutions to Schrödinger's equation for the hydrogen atom gives a set of wave functions w/ corresponding energies. The wave functions are orbitals.

- Each orbital describes a specific distribution of e⁻ density & has a characteristic shape.

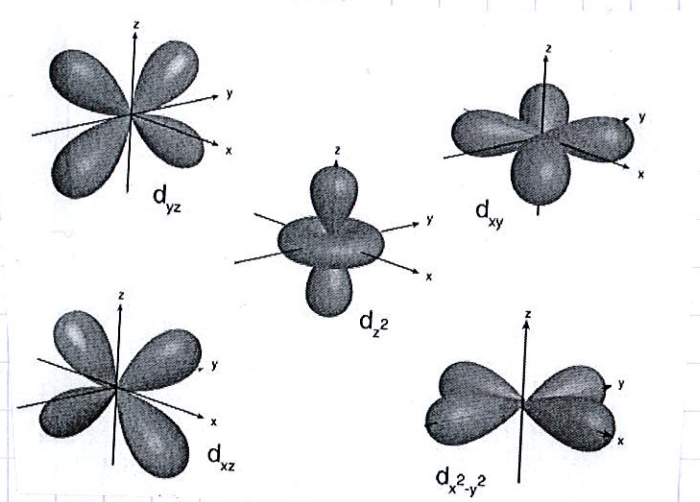
1) The s orbitals - spherical



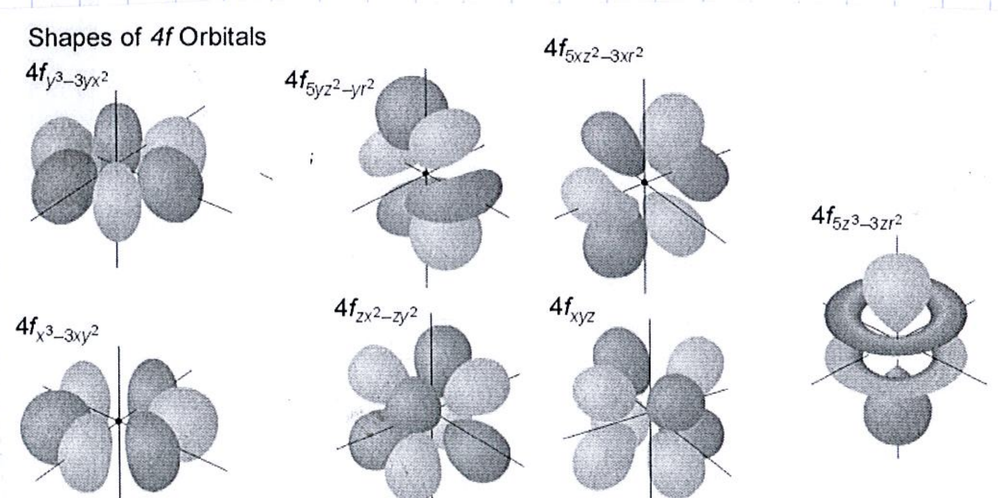
2) The p orbitals - teardrops/infinity shape



3) The d orbitals



4) The f orbitals



n=4 has 4 sublevels – add f orbitals

Seven f orbitals in every energy level from n=4 to n=∞:

4f, 5f, 6f ... (don't need to know shapes)

Every new sublevel will add 2 more orbitals

6. Electron Configurations & Orbital Diagrams

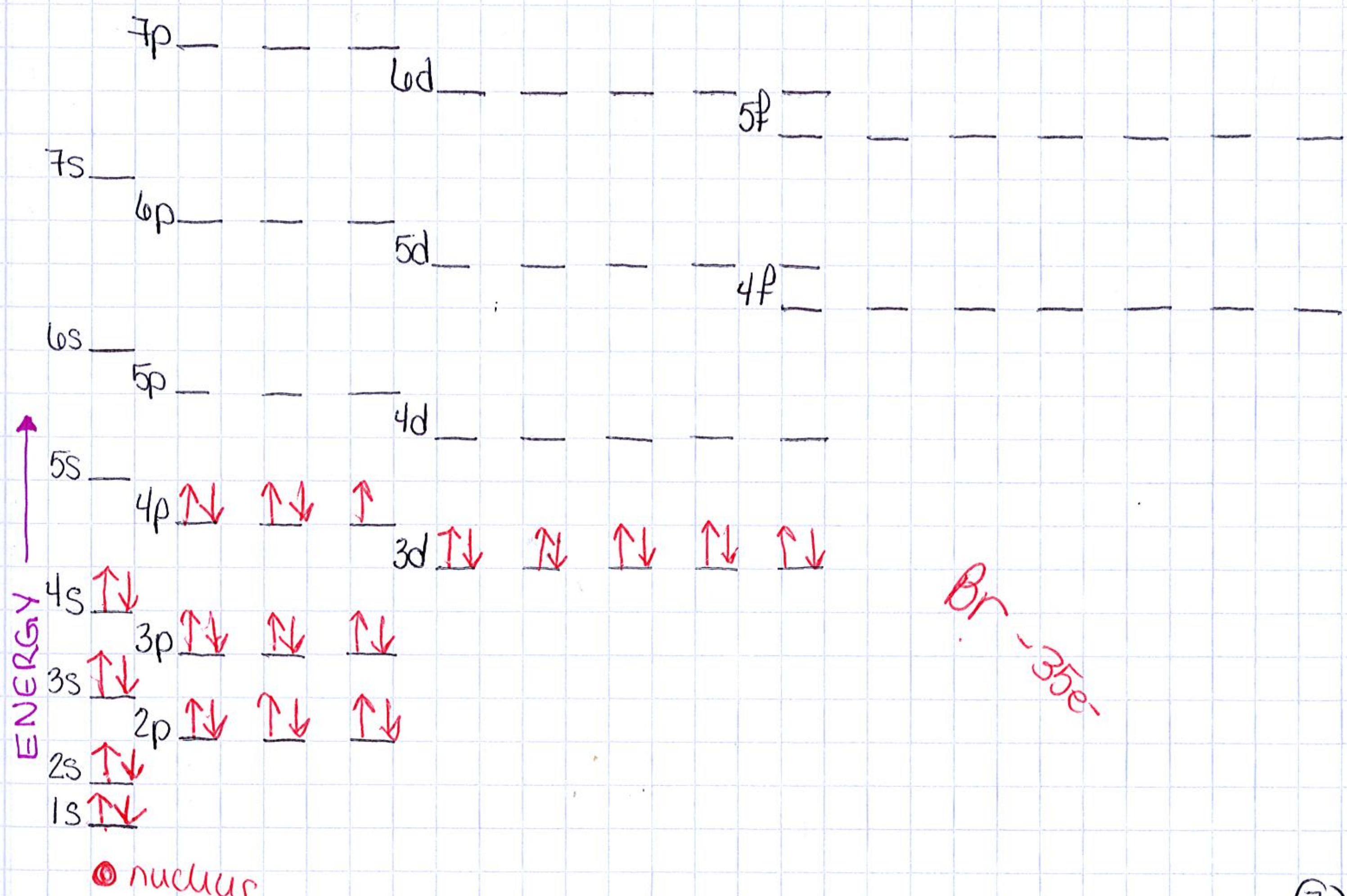
Both orbital diagrams & electron configurations show the distribution of all the electrons in an atom into its orbitals

A) Ground state - shows e⁻ in the lowest possible energy states (closest to the nucleus)

B) Some rules we must follow:

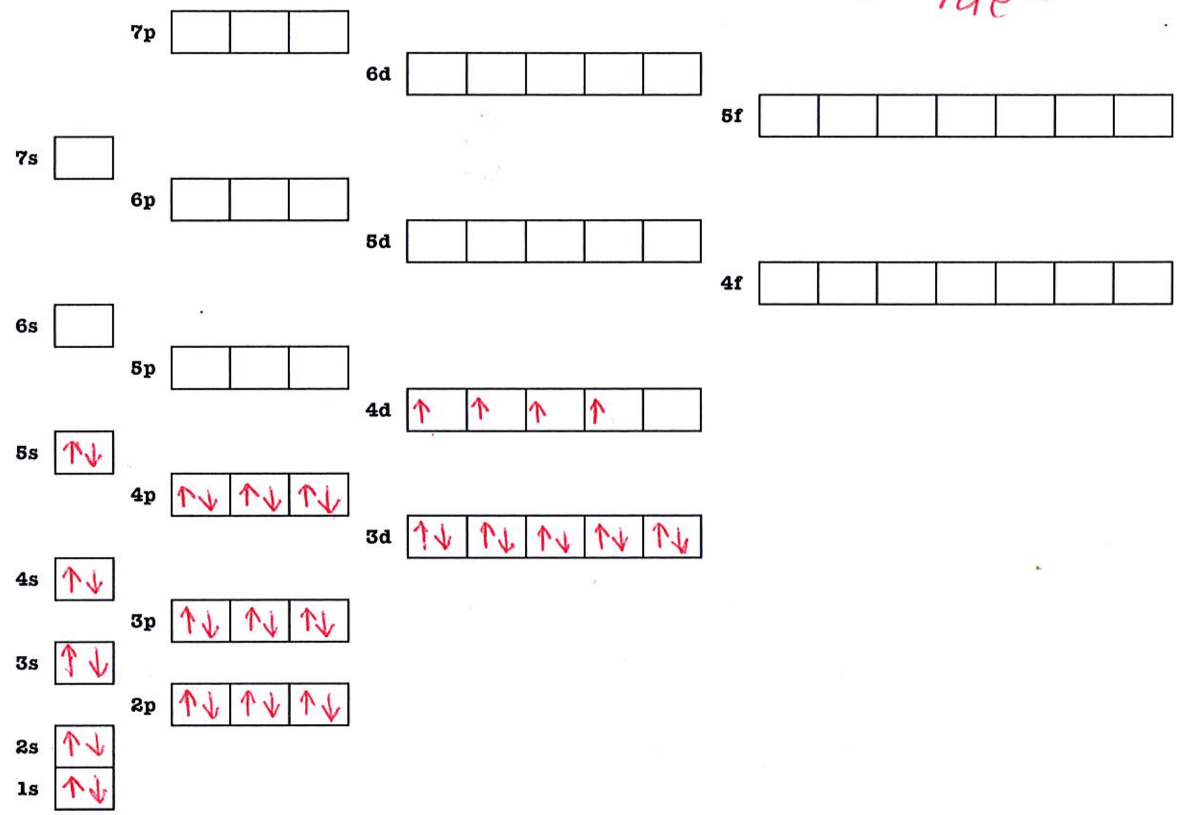
1) 2 e⁻ can exist within one orbital, as long as they spin in opposite directions (electron spin)
   Pauli Exclusion Principle
2) Orbitals are filled in order of increasing energy, with one e⁻ filling orbitals of the same energy before a second e⁻ can enter an orbital.
   Hund's Rule

C) Orbital Diagrams

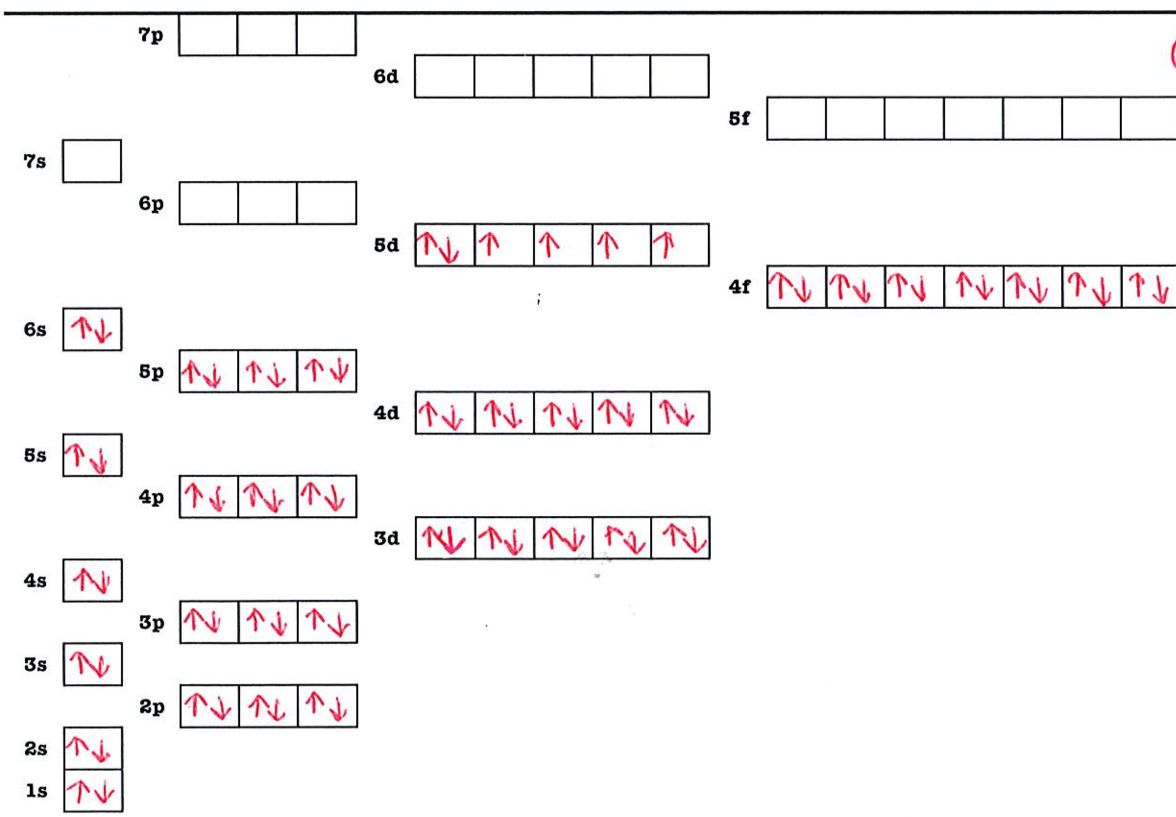


Examples - Orbital Diagrams

Mo - 42e-

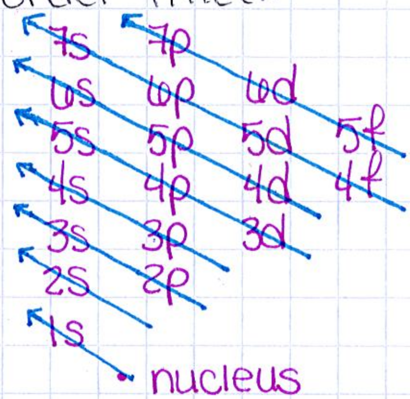


Os - 76e-



D. Electron configurations - show the order in written format

1) order filled.



s = 2e-
p = 6e-
d = 10e-
10 = 14e-

Examples

13) Si - 14e-

$1s^2 2s^2 2p^6 3s^2 3p^2$

14) Ti 22e-

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$

15) As - 33e-

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
$3d^{10} 4p^3$

16) Sr - 38e-

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$
$4p^6 5s^2$

2) Exceptions - Elements in group 6 & group 11

A) Group 6 - Rather than having the "d" block have 4e- in in, one e- from s orbital joins the "d" orbital so it is ½ filled

- Cr & Mo

Cr - $1s^2 2s^2 2p^6 3s^2 3p^6$ <u>$4s^1 3d^5$</u>

Mo - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$ <u>$5s^1 4d^5$</u>

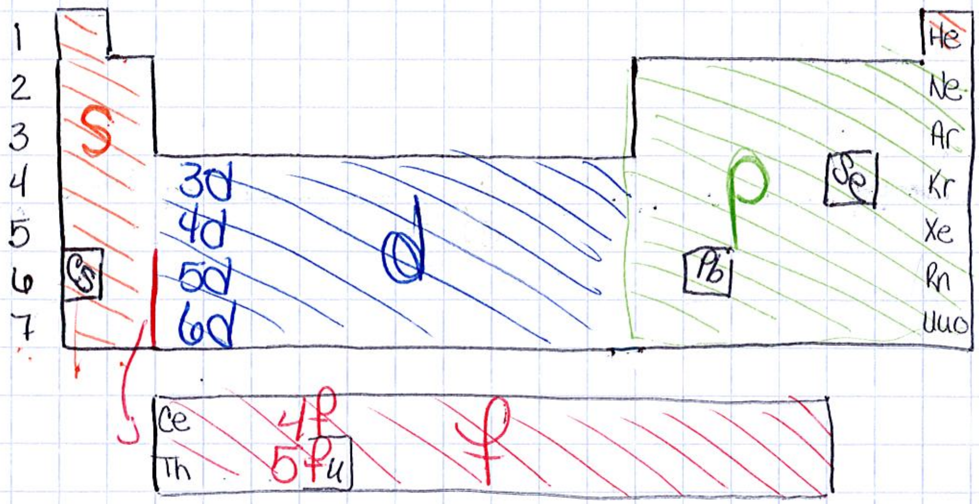
B) Group 11 - fills the d orbital completely by taking 1e- from the s orbital

Cu - $1s^2 2s^2 2p^6 3s^2 3p^6$ <u>$4s^1 3d^{10}$</u>

Ag - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$ <u>$5s^1 4d^{10}$</u>

Au - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10}$ <u>$6s^1 4f^{14} 5d^{10}$</u>

4) Using the Periodic Table & Noble Gas configurations



Examples

17) Cs $[Xe]6s^1$

18) Se $[Ar]4s^2 3d^{10} 4p^4$

19) Pb $[Xe]6s^2 4f^{14} 5d^{10} 6p^2$

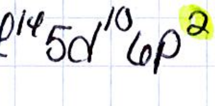
20) U $[Rn]7s^2 5f^4$

A) Valence e^- = e^- in the highest energy level
Core e^- = all other e^-

E. Electron Spin & magnetism

1) magnetism - force of repulsion/attraction between 2 like/un-like poles

- e^-, in most atoms, exist in pairs with each e^- spinning in opposite directions



each spinning e^- causes a magnetic field to form around it.

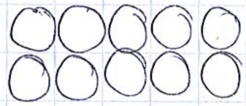
when paired up, the opposing magnetic fields cancel each other out.

A magnetic moment!

when there are unpaired e^-, like in Fe, Co, & Ni, the magnetic field does NOT cancel out & each atom acts like a tiny magnet!

4) Types of magnetism

A) diamagnetic matter - no unpaired e^-; weakly repelled by a magnet



B) paramagnetic matter - has at least 1 unpaired e^-. Attracted to magnets. Each magnetic moment is not aligned to others near it

c) ferromagnetic matter - occurs when unpaired e^- are affected by the orientation of other e^- around it.
Only Fe, Co, & Ni are ferromagnetic!

stronger than paramagnetism!

Example

21) which of the following are expected to be diamagnetic? paramagnetic?

He	Be	Li	N
$1s^2$	$1s^2 2s^2$	$1s^2 2s^1$	$1s^2 2s^2 2p^3$
dia	dia	para	para

N: 2p ↑ ↑ ↑

O

$1s^2 2s^2 2p^4$

2p ↑↓ ↑ ↑

para